Dimer radical cations of Indole and Indole-3-carbinol. Localized and delocalized radical cations of Diindolylmethane.

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Supporting Information

Note : the geometries and energies of all stationary points mentioned in the paper, and the detailed results of excited state calculations are provided in a separate text file

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Complete citation of the Gaussian program :

Frisch, M.J.T., G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Scalmani, G.; Barone, V.; Mennucci, B.; Petersson, G. A.; Nakatsuji, H.; Caricato, M.; Li, X.; Hratchian, H. P.; Izmaylov, A. F.; Bloino, J.; Zheng, G.; Sonnenberg, J. L.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Vreven, T.; Montgomery, Jr., J. A.; Peralta, J. E.; Ogliaro, F.; Bearpark, M.; Heyd, J. J.; Brothers, E.; Kudin, K. N.; Staroverov, V. N.; Kobayashi, R.; Normand, J.; Raghavachari, K.; Rendell, A.; Burant, J. C.; Iyengar, S. S.; Tomasi, J.; Cossi, M.; Rega, N.; Millam, N. J.; Klene, M.; Knox, J. E.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Martin, R. L.; Morokuma, K.; Zakrzewski, V. G.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Dapprich, S.; Daniels, A. D.; Farkas, Ö.; Foresman, J. B.; Ortiz, J. V.; Cioslowski, J.; Fox, D. J., *Gaussian 09, Rev. A02*, Gaussian, Inc., Wallingford CT, **2009**.

Table S1. Excited states of $(I3C)_2^{\bullet+}$ (conformer ***B***) calculated by TD-B2PLYPD/cc-pVDZ

Excited state	*Energy* eV	nm	*Oscillator strength*	*Main excitation*	
1st	1.38	902	0.0001	75β → 78β	0.74592
2nd	1.49	830	0.0018	77β → 78β	0.81770
3rd	1.93	642	0.0042	76β → 78β	0.94639
4th	**2.60**	**477**	**0.0721**	**73β → 78β**	**0.93682**
5th	2.61	476	0	highly mixed	
6th	3.58	347	0.025	highly mixed	
7th	3.58	346	0.003	74β → 78β	0.96707
8th	3.84	323	0.0001	highly mixed	

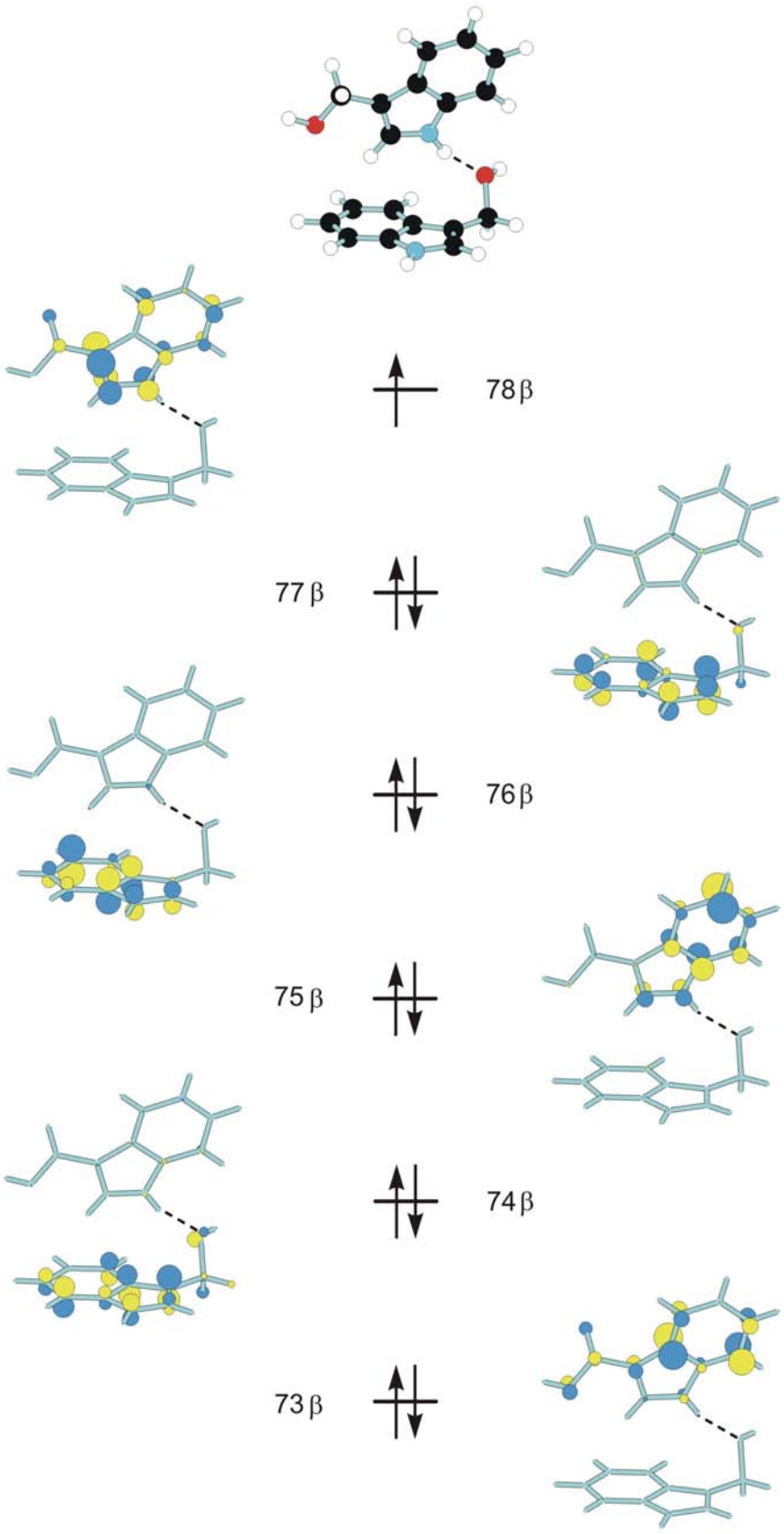

Figure S1. KS molecular orbitals of $(I3C)_2^{\bullet+}$ (conformer ***B***) involved in the electronic transitions of these species (cf. **Table 1**).

Table S2. Equilibrium conformations of **DIM** and its radical cations by B2-PLYP-D/cc-pVDZ.

	B2PLYPD/cc-pVDZ				
	d_1	d_2	E_{rel}	G_{rel}^*	H_{rel}^*
C_1	5	-116	0.00	0.00	0.00
C_2	128	128	0.26	0.84	0.27
C_S	76	-92	0.25	0.21	0.24
C_2-a	147	147	1.28	1.89	0.98
C_2-b	68	68	0.00	0.00	0.00

calculated by the B2PLYP-D/cc-pVDZ method, using B3LYP/6-31G thermal corrections and entropies.

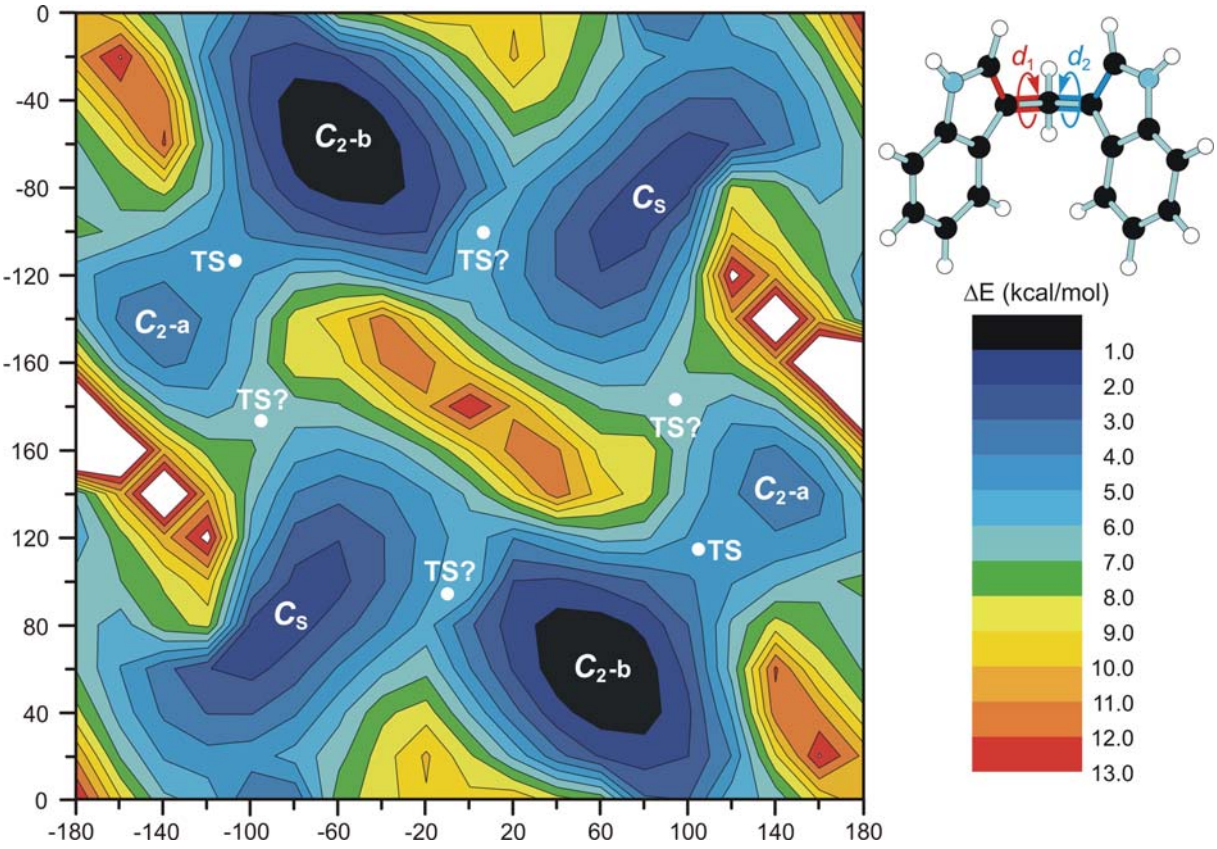

Figure S2. B3LYP/6-31G*.potential energy surface generated by scanning the two dihedral angles d_1 and d_2, in **DIM**$^{\bullet+}$